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We consider estimation of a variance function g in regression problems. Such estimation requires simultaneous estimation of the mean function f. We obtain sharp results on the extent to which the smoothness of f influences best rates of convergence for estimating g. For example, in nonparametric regression with two derivatives on g, "classical" rates of convergence are possible if and only if the unknown f satisfies a Lipschitz condition of order $\frac{1}{3}$ or more. If a parametric model is known for g, then g may be estimated $n^{\frac{1}{2}}$ - consistently if and only if f is Lipschitz of order $\frac{1}{4}$ or more. Optimal rates of convergence are attained by kernel estimators. (KR)


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# Variance Function Estimation in Regression:
# The Effect of Estimating the Mean

Technical Report #4

Peter Hall and R. J. Carroll

# Variance Function Estimation in Regression:

# The Effect of Estimating the Mean

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## SUMMARY

We consider estimation of a variance function $g$ in regression problems. Such estimation requires simultaneous estimation of the mean function $f$. We obtain sharp results on the extent to which the smoothness of $f$ influences best rates of convergence for estimating $g$. For example, in nonparametric regression with two derivatives on $g$, "classical" rates of convergence are possible if and only if the unknown $f$ satisfies a Lipschitz condition of order $\frac{1}{3}$ or more. If a parametric model is known for $g$, then $g$ may be estimated $n^{\frac{1}{2}}$-consistently if and only if $f$ is Lipschitz of order $\frac{1}{2}$ or more. Optimal rates of convergence are attained by kernel estimators.

Keywords: Heteroscedasticity; Nonparametric Regression; Rates of Convergence; Variance Functions.

## 1. INTRODUCTION

Consider a heteroscedastic regression problem of the form

$$Y_i = f(x_i) + g(x_i)^{\frac{1}{2}} \epsilon_i \,, \quad 1 \le i \le n \,, \tag{1.1}$$

where the design variables $x_i$ may be either regularly or randomly spaced, and where the $\epsilon_i$'s are independent with zero mean and unit variance. Estimation of the variance function $g$ is important in many contexts. Besides the classic need to estimate variance so as to compute weighted least squares estimates of the mean function $f$, variance function estimates are needed in quality control (Box & Ramirez, 1987); immunoassay (Butt, 1984); prediction, where knowledge of $g$ is required to supply confidence intervals for $f$ (Carroll, 1987); calibration (Watters, Spiegelman & Carroll, 1987); and the estimation of detection limits (Carroll, Davidson & Smith, 1987). These applications are discussed in detail by Carroll & Ruppert (1988). In the present paper we provide a concise description of the effect which not knowing $f$ has on estimation of $g$.

The results are curious and unexpected. For example, if $f$ is not known parametrically but has at least half a derivative (i.e. satisfies a Lipschitz condition of order $\frac{1}{2}$ or more), then $g$ can be estimated with an accuracy which would be optimal if $f$ were completely known. This result applies to problems where $g$ is known parametrically, and also to problems where $g$ must be estimated nonparametrically. However, the result fails if $f$ is so rough that it does not have half a derivative. There, the roughness of $f$ completely determines the convergence rate if $g$ has known parametric form, and influences the rate if $g$ is known nonparametrically. These remarks apply to optimal estimators of $g$, as well as to kernel estimators. We show that kernel estimators achieve best possible rates of convergence.

In more detail, the fastest achievable $L^2$ rate of convergence is

$$\max\left(n^{-2\nu_2/(2\nu_2+1)}, n^{-4\nu_1/(2\nu_1+1)}\right) \tag{1.2}$$

if $f$ has $\nu_1$ derivatives and $g$ has $\nu_2$ derivatives. If $\nu_1 \geq \frac{1}{2}$, this equals $n^{-2\nu_2/(2\nu_2+1)}$ and so does not depend on $\nu_1$. Rates in the case where $g$ is known parametrically may be obtained by taking $\nu_2 = \infty$ in (1.2), in which event (1.2) becomes $\max(n^{-1}, n^{-4\nu_1/(2\nu_1+1)})$. The latter equals $n^{-1}$ if $\nu_1 \geq \frac{1}{2}$.

Section 2 presents these conclusions in detail for the case where design points $x_i$ in (1.1) are regularly spaced. Section 3 outlines analogous results for the case of random designs.

## 2. REGULAR DESIGN

**2.1 Introduction.** In this section we take the model to be

$$Y_i = f(i/n) + g(i/n)^{\frac{1}{2}}\epsilon_i\,, \quad 1 \leq i \leq n\,, \tag{2.1}$$

where $f$ and $g$ are bounded functions on the interval [0,1], $g \geq 0$, and $\epsilon_1, \epsilon_2, \ldots$ are independent random variables with zero mean, unit variance and uniformly bounded fourth moment. Given $\nu > 0$, write $\langle\nu\rangle$ for the largest integer strictly less than $\nu$. We say that a function $a$, such as $f$ or $g$, is $\nu$-smooth if (i) derivatives $a^{(0)}, \ldots, a^{(\langle\nu\rangle)}$ exist and are bounded on [0,1]; and (ii) $a^{(\langle\nu\rangle)}$ satisfies a Lipschitz condition of order $\nu - \langle\nu\rangle$ on [0,1]:

$$|a^{(\langle\nu\rangle)}(x) - a^{(\langle\nu\rangle)}(y)| \leq C|x-y|^{\nu-\langle\nu\rangle}\,, \quad \text{all } x, y \in [0,1]\,.$$

A function with $k$ bounded derivatives on [0,1] is $k$-smooth.

In subsection 2.2 we show that if $f$ is $\nu_1$-smooth and $g$ is $\nu_2$-smooth, then kernel-type estimators of $g$ converge in mean square at rate $\max(n^{-2\nu_2/(2\nu_2+1)}, n^{-4\nu_1/(2\nu_1+1)})$. Subsection 2.3 demonstrates that if the errors $\epsilon_i$ are Gaussian then this rate is optimal, in the sense that no estimator can converge to $g$ more rapidly in mean square. Subsection 2.4 treats the case $\nu_2 = \infty$, which amounts to postulating a parametric model for $g$.

**2.2 Kernel-type estimators.** We begin by defining an analogue of a kernel sequence for regular designs. Suppose $0 < h \leq 1$, and $m \geq 0$ is an integer. Let $c_k = c_k(h, m)$,

$-\infty < k < \infty$, be constants satisfying

$$|c_k| \leq Ch, c_k = 0 \quad \text{for} \quad |k| \geq Ch^{-1}, \quad \Sigma_k c_k = 1$$
$$\text{and} \quad \Sigma_k k^i c_k = 0 \quad \text{for } 1 \leq i \leq m, \tag{2.2}$$

where the constant $C$ does not depend on $h$. Then $\Sigma_k |k|^\alpha |c_k| \leq 2C^{\alpha+2} h^{-\alpha}$ for each $\alpha \geq 0$, and $\Sigma_k c_k^2 \leq 2C^3 h$. The $c_k$'s may be constructed starting from a smooth function $K$, vanishing outside the interval $[-1,1]$ and satisfying $\int K(x)\,dx = 1$, $\int x^i K(x)\,dx = 0$ for $1 \leq i \leq m$. Minor adjustments to $K$, giving a new function $K_1$ say, ensure that at least for small $h$, $c_k = hK_1(hk)$ yields an appropriate sequence of constants. For example, if $m = 0$ or 1, take $K$ to be a bounded, continuous density, symmetric about the origin and vanishing outside $[-1,1]$. Define $\kappa(h)$ by $\kappa(h)^{-1} \equiv \Sigma_k hK(hk)$, so that $\kappa(h) \to 1$ as $h \to 0$. Then $c_k \equiv \kappa(h)hK(hk)$ satisfies our conditions on $c_k$.

Next we define an estimator of $f$. Suppose the data $Y_i$, $1 \leq i \leq n$, are generated by model (2.1). If the mean function $f$ is $\nu_1$-smooth, choose a sequence of constants $a_k \equiv c_k(h_1, \langle \nu_1 \rangle)$ satisfying condition (2.2), and put

$$\hat{f}(i/n) \equiv \Sigma_k a_k Y_{i+k}, \quad 0 \leq i \leq n, \tag{2.3}$$

where $Y_j$ is defined to be zero if $j < 1$ or $j > n$. Use linear interpolation on $\hat{f}(i/n)$ to construct $\hat{f}(x)$ for general $x \in [0,1]$. We show in Appendix (i) that if $f$ is $\nu_1$-smooth and $g$ is bounded, and if $h_1 \to 0$ and $nh_1 \to \infty$ as $n \to \infty$, then for each $0 < \delta < \frac{1}{2}$,

$$\sup_{\delta \leq x \leq 1-\delta} |E\hat{f}(x) - f(x)| = O\{(nh_1)^{-\nu_1}\}, \tag{2.4}$$
$$\sup_{\delta \leq x \leq 1-\delta} \operatorname{var}\{\hat{f}(x)\} = O(h_1). \tag{2.5}$$

Therefore the mean squared error of $\hat{f}$ satisfies

$$\sup_{\delta \leq x \leq 1-\delta} E\{\hat{f}(x) - f(x)\}^2 = O\{h_1 + (nh_1)^{-2\nu_1}\}, \tag{2.6}$$

which is minimized at $O(n^{-2\nu_1/(2\nu_1+1)})$ by choosing $h_1$ to be of size $n^{-2\nu_1/(2\nu_1+1)}$.

Now we construct estimators of $g$. The estimated residuals are

$$\hat{r}_i \equiv Y_i - \hat{f}(i/n), \quad 1 \leq i \leq n .$$

Our hope is that $\hat{r}_i$ will be close to the "true" residual, $r_i \equiv Y_i - f(i/n) = g(i/n)^{\frac{1}{2}}\epsilon_i$. (Define $r_i = \hat{r}_i = 0$ if $i < 1$ or $i > n$.) Of course, $r_i^2$ admits the model type (2.1):

$$r_i^2 = g(i/n) + g(i/n)\eta_i , \quad 1 \leq i \leq n , \tag{2.7}$$

where $\eta_i^2 \equiv \epsilon_i^2 - 1$ are independent and identically distributed with zero mean. If the $r_i$'s were observable, we could estimate $g$ from $\{r_i^2\}$ in exactly the same way that we estimated $f$ from $\{Y_i\}$: assuming $g$ to be $\nu_2$-smooth, choose a sequence of constants $b_k \equiv c_k(h_2, (\nu_2))$ satisfying (2.2), and put

$$\tilde{g}(i/n) \equiv \Sigma_k b_k r_{i+k}^2 , \quad 1 \leq i \leq n .$$

Construct $\tilde{g}(x)$ by linear interpolation. We see directly from (2.6) that if $h_2 \to 0$ and $nh_2 \to \infty$ then

$$\sup_{\delta \leq x \leq 1-\delta} E\{\tilde{g}(x) - g(x)\}^2 = O\{h_2 + (nh_2)^{-2\nu_2}\} . \tag{2.8}$$

Of course, $\tilde{g}$ is not a realistic estimator, since the true residuals are not observable. If we replace true residuals by their estimates we obtain the practical estimator,

$$\hat{g}(i/n) \equiv \Sigma_k b_k \hat{r}_{i+k}^2 , \quad 1 \leq i \leq n . \tag{2.9}$$

Construct $\hat{g}(x)$ by linear interpolation. We show in Appendix (ii) that for each $0 < \delta < \frac{1}{2}$,

$$\sup_{\delta \leq x \leq 1-\delta} E\{\hat{g}(x) - g(x)\}^2 = O\left[\{h_2 + (nh_2)^{-2\nu_2}\} + \{h_1 + (nh_1)^{-2\nu_1}\}^2\right] . \tag{2.10}$$

The second term on the right-hand side of (2.10) distinguishes that expression from (2.8), and is a consequence of our imperfect knowledge about $f$. Notice that it is the square of the right-hand side of (2.6).

To optimize the rate at which the right-hand side of (2.10) converges to zero, choose $h_i$ of size $n^{-2\nu_i/(2\nu_i+1)}$ for $i = 1$ and 2. Then

$$\sup_{\delta \leq x \leq 1-\delta} E\{\hat{g}(x) - g(x)\}^2 = O\{\max(n^{-2\nu_2/(2\nu_2+1)}, n^{-4\nu_1/(2\nu_1+1)})\} . \tag{2.11}$$

A necessary and sufficient condition for the term in $\nu_2$ here to dominate, is $4\nu_1/(2\nu_1+1) \geq 2\nu_2/(2\nu_2+1)$, or equivalently,

$$\nu_1 \geq \nu_2/\{2(\nu_2+1)\} . \tag{2.12}$$

Should this condition fail, the rate of convergence of $\hat{g}$ to $g$ is limited by smoothness (or more correctly, lack of smoothness) of $f$, not by smoothness of $g$. On the other hand, if (2.12) holds then the rate of convergence of $\hat{g}$ to $g$ is determined by smoothness of $g$. Note that $\nu_2/\{2(\nu_2+1)\} < \frac{1}{2}$ for all $\nu_2 > 0$, and so condition (2.12) is assured if $\nu_1 \geq \frac{1}{2}$ — that is, if $f$ has at least "half a derivative".

**2.3 Optimal rates of convergence.** Let $C(\nu, B)$ denoted the class of $\nu$-smooth functions $a : [0,1] \to \mathbb{R}$, such that $\sup |a^{(j)}| \leq B$ for $0 \leq j \leq \langle\nu\rangle$ and

$$|a^{(\langle\nu\rangle)}(x) - a^{(\langle\nu\rangle)}(y)| \leq B|x-y|^{\nu - \langle\nu\rangle} , \quad \text{all } x, y \in [0,1] .$$

Write $C_+(\nu, B)$ for the set of $a \in C(\nu, B)$ with $a \geq 0$. We showed in Subsection 2.1 that if $f \in C(\nu_1, B)$ and $g \in C_+(\nu_2, B)$, then we may construct a nonparametric estimator $\hat{g}$ of $g$ such that

$$\sup_{\delta \leq x \leq 1-\delta} E\{\hat{g}(x) - g(x)\}^2 = O\{\max(n^{-2\nu_2/(2\nu_2+1)}, n^{-4\nu_1/(2\nu_1+1)})\}$$

for each $\delta \in (0, \frac{1}{2})$. See (2.11). It is a simple matter to sharpen our proof of this result so that it applies uniformly in $f$ and $g$:

$$\sup_{f \in C(\nu_1, B), g \in C_+(\nu_2, B)} \ \sup_{\delta \leq x \leq 1-\delta} E_{f,g}\{\hat{g}(x) - g(x)\}^2 = O\{\max(n^{-2\nu_2/(2\nu_2+1)}, n^{-4\nu_1/(2\nu_1+1)})\}.$$

We claim that this rate of convergence is best possible, in the following sense. If $\hat{g}$ is *any* nonparametric estimator of $g$, if $0 < x_0 < 1$, and if the errors $\epsilon_i$ are Gaussian, then for some $C > 0$ and all sufficiently large $n$,

$$M \equiv \sup_{f\in\mathcal{C}(\nu_1,B),g\in\mathcal{C}_+(\nu_2,B)} E_{f,g}\{\hat{g}(x_0)-g(x_0)\}^2 \geq C\max(n^{-2\nu_2/(2\nu_2+1)}, n^{-4\nu_1/(2\nu_1+1)}). \tag{2.13}$$

This statement is a combination of two results, declaring that

$$M_n \geq Cn^{-2\nu_2/(2\nu_1+1)} \tag{2.14}$$

and

$$M_n \geq Cn^{-4\nu_1/(2\nu_1+1)} \tag{2.15}$$

respectively. The first of these inequalities has a relatively simple proof, which we now outline. Take $f \equiv 0$, so that we observe the "true" residuals $r_i \equiv g(i/n)^{\frac{1}{2}}\epsilon_i$. The sequence $r_1^2, \ldots, r_n^2$ is sufficient for $g$. Therefore the problem is that of estimating $g$ under model (2.7). Techniques described by Stone (1980) are easily modified to produce the inequality

$$\sup_{g\in\mathcal{C}_+(\nu_2,B)} E_g\{\hat{g}(x_0)-g(x_0)\}^2 \geq Cn^{-2\nu_2/(2\nu_2+1)},$$

where $\hat{g}$ is any nonparametric estimator of $g$ based on $r_1^2, \ldots, r_n^2$, and where $f \equiv 0$. This gives (2.14). Appendix (iii) presents a proof of (2.15).

**2.4 Parametric model for variance.** In some circumstances it is appropriate to consider a parametric model for $g$, such as $g(x) \equiv \exp(cx+d)$. As far as rates of convergence go, this amounts to taking $\nu_2 = \infty$ in the preceding work, as we now relate.

Suppose $g$ has known parametric form. If $f$ were available we could compute the "true" residuals $r_i \equiv Y_i - f(i/n)$, and from them compute an estimator $\tilde{g}$ satisfying $E\{\tilde{g}(x)-g(x)\}^2 = O(n^{-1})$. More practically, assume $f$ is $\nu_1$-smooth and compute our kernel-type estimator $\hat{f}$, defined at (2.3). Calculate the estimated residuals $\hat{r}_i \equiv Y_i - \hat{f}(i/n)$. Since the constants $a_k$ in (2.3) vanish for $|k| \geq Ch_1^{-1}$ (see (2.2)), we avoid "edge effects" by using only those $\hat{r}_i$'s with $Ch_1^{-1} \le i \le n - Ch_1^{-1}$. Modify $\hat{g}$ by (i) including only these indices $i$, and (ii) replacing $r_i$ by $\hat{r}_i$. Call the new estimator $\hat{g}$. Then for each $0 < \delta < \frac{1}{2}$,

$$\sup_{\delta \le x \le 1-\delta} E\{\hat{g}(x) - g(x)\}^2 = O\left[n^{-1} + \{h_1 + (nh_1)^{-2\nu_1}\}^2\right] . \tag{2.16}$$

This is an analogue of (2.10). To optimize the rate of convergence of the right-hand side, choose $h_1$ to be of size $n^{-2\nu_1/(2\nu_1+1)}$, obtaining

$$\sup_{\delta \le x \le 1-\delta} E\{\hat{g}(x) - g(x)\}^2 = O\{\max(n^{-1}, n^{-4\nu_1/(2\nu_1+1)})\} . \tag{2.17}$$

This is just (2.11) with $\nu_2 = \infty$.

A necessary and sufficient condition for the $n^{-1}$ term to dominate the right-hand side of (2.17), is $\nu_1 \ge \frac{1}{2}$; this is just (2.12) with $\nu_2 = \infty$. If $\nu_1 < \frac{1}{2}$, or equivalently if $f$ has "less than half a derivative", then estimation of even a parametric $g$ is a nonparametric problem with nonparametric rates of convergence. When $\nu_1 = \frac{1}{2}$, $E\{\hat{g}(x) - g(x)\}^2 = O(n^{-1})$, although constants $C_1$ and $C_2$ in asymptotic formulae such as

$$E\{\tilde{g}(x) - g(x)\}^2 \sim C_1(x)n^{-1} , \quad E\{\hat{g}(x) - g(x)\}^2 \sim C_2(x)n^{-1}$$

can differ. But when $\nu_1 > \frac{1}{2}$, our imperfect knowledge about $f$ vanishes from the asymptotics, and

$$E\{\tilde{g}(x) - g(x)\}^2 = \{1 + o(1)\}E\{\hat{g}(x) - g(x)\}^2 = O(n^{-1}) \tag{2.18}$$

as $n \to \infty$. (This result has an analogue in the nonparametric case, when $\nu_1 > \nu_2/\{2(\nu_2 + 1)\}$.)

It is tedious to verify all these formulae in the general case, owing to the wide variety of possible parametric models and associated estimators. We treat only the case $g = g(x) \equiv \sigma^2$ (constant) on [0,1]. Here, $\tilde{g} \equiv n^{-1}\Sigma_{1 \le i \le n} r_i^2$ and, with $m$ denoting the smallest integer greater than $Ch_1^{-1}$,

$$\hat{g} \equiv (n - 2m)^{-1} \sum_{i=m}^{n-m+1} \hat{r}_i^2 = (n - 2m)^{-1} \sum_{i=m}^{n-m+1} r_i^2 + (n - 2m)^{-1} \sum_{i=m}^{n-m+1} \{\hat{f}(i/n) - f(i/n)\}^2 + 2g^{\frac{1}{2}}(n - 2m)^{-1} \sum_{i=m}^{n-m+1} \epsilon_i\{f(i/n) - \hat{f}(i/n)\} .$$

Writing $B_i \equiv E\hat{f}(i/n) - f(i/n)$ for bias, and $\tilde{g}_m \equiv (n-2m)^{-1}\Sigma_{m\leq i\leq n-m+1} r_i^2$, we obtain

$$(\hat{g} - \tilde{g}_m)^2 \leq Cn^{-2}\Bigg[\Bigg(\sum_{i=m}^{n-m+1} B_i^2\Bigg)^2 + \Bigg\{\sum_{i=m}^{n-m+1} (\Sigma_k a_k \epsilon_{i+k})^2\Bigg\}^2 + \Bigg(\sum_{i=m}^{n-m+1} B_i\epsilon_i\Bigg)^2 + \Bigg\{\sum_{i=m}^{n-m+1} \epsilon_i(\Sigma_k a_k \epsilon_{i+k})\Bigg\}^2\Bigg].$$

Now, $|B_i| = O\{(nh_1)^{-2\nu_1}\}$ uniformly in $m \leq i \leq n-m+1$, and so

$$E(\hat{g} - \tilde{g}_m)^2 = O\big[\{h_1 + (nh_1)^{-2\nu_1}\}^2\big] + o(n^{-1}).$$

Results (2.16)–(2.18) follow from this formula.

The lower bound (2.13), this time with $\nu_2 = \infty$, continues to hold in parametric circumstances such as the one above. In fact, our proof of (2.13) in Appendix (iii) is applicable to the parametric case.

## 3. RANDOM DESIGN

We now consider kernel regression estimators in the random design case. Let $h$ be the density of the design. Typically, when $h$ is known it is relatively easy to show that the $L^2$ rate of convergence satisfies (1.2). We concentrate instead on the case of an unknown design density. Under (2.12), we show that one can estimate the variance function $g$ as accurately as though $f$ were known.

Observe independent pairs $(Y_i, x_i)$, $1 \leq i \leq n$. The $x_i$'s have common density $h$, and given $\{x_i\}$, $Y_i = f(x_i) + g(x_i)^{\frac{1}{2}}\epsilon_i$. The $\epsilon_i$'s are assumed to have mean zero, variance one, and uniformly bounded fourth moments. Given $\nu > 0$, define $\langle\nu\rangle$ and "$\nu$-smoothness" as in Subsection 2.1. Assume $f$ is $\nu_1$-smooth and $g$ is $\nu_2$-smooth, where $\nu_1 > 0$ and $\nu_2 > 0$. Suppose that, uniformly in a neighborhood of $x_0$, the density $d$ of $x$ is $\{\max(\nu_1, \nu_2)\}$-smooth and bounded away from zero and infinity. For $j = 1, 2$, let $K_j$ be continuous functions with support $[-1, 1]$, integrating to one, uniformly Lipschitz continuous of order one, and with $i$'th moment equal to zero for $1 \leq i \leq \langle\nu_j\rangle$. Let $h_j \equiv n^{-1/(2\nu_j+1)}$ for $j = 1, 2$.

Define

$$\hat{d}_j(x) \equiv (nh_j)^{-1} \sum_{k=1}^{n} K_j\{(x_k - x)/h_j\}\,, \quad \hat{d}_{1i}(x) \equiv (nh_1)^{-1} \sum_{k \neq i} K_1\{(x_k - x)/h_1\}\,.$$

A kernel regression estimator of $f$ is

$$\hat{f}_i(x) \equiv (nh_1)^{-1} \sum_{k \neq i} Y_k K\{(x_k - x)/h_1\}/\hat{d}_{1i}(x)\,.$$

If the mean function $f$ were known, a kernel regression estimator of $g$ would be

$$\tilde{g}(x) \equiv (nh_2)^{-1} \sum_{i=1}^{n} \{Y_i - f(x_i)\}^2 K_2\{(x_i - x)/h_2\}/\hat{d}_2(x)\,.$$

If $f$ is unknown, the natural analogue of $\tilde{g}$ is

$$\hat{g}(x) \equiv (nh_2)^{-1} \sum_{i=1}^{n} \{Y_i - \hat{f}_i(x_i)\}^2 K_2\{(x_i - x)/h_2\}/\hat{d}_2(x)\,.$$

Classical results on kernel regression function estimation may be used to prove that $|\tilde{g}(x_0) - g(x_0)| = O_p(n^{-\nu_2/(2\nu_2+1)})$; this is the analogue of (2.8) for an optimal choice of window size $h_2$. In analogy with (2.11),

$$|\hat{g}(x_0) - g(x_0)| = O_p\{\max(n^{-\nu_2/(2\nu_2+1)}\,,\, n^{-2\nu_1/(2\nu_1+1)})\}\,. \tag{3.1}$$

As in Section 2, a necessary and sufficient condition for the term in $\nu_2$ here to dominate, is $\nu_1 \geq \nu_2/\{2(\nu_2 + 1)\}$. If this inequality is strict then $\hat{g}$ is asymptotically equivalent to the "ideal" estimator $\tilde{g}$, in the sense that

$$|\hat{g}(x_0) - \tilde{g}(x_0)| = o_p(n^{-\nu_2/(2\nu_2+1)})\,. \tag{3.2}$$

To prove (3.2), first observe from Stute (1984) that

$$\sup_{|x-x_0|\leq c} \{|\hat{d}_j(x) - d(x)|\} = O_p(n^{-\nu_j/(2\nu_j+1)} \log n)$$

for some $c > 0$. From this it follows that

$$\sup_{|x-x_0|\leq c} \max_{1\leq i\leq n} |\hat{d}_{1i}(x) - d(x)| = O_p(n^{-\nu_1/(2\nu_1+1)} \log n)\,. \tag{3.3}$$

Therefore to prove (3.2) it suffices to show that

$$\max(|A_n|, |B_n|) = o_p(n^{-\nu_2/(2\nu_2+1)}) , \tag{3.4}$$

where

$$A_n \equiv (nh_2)^{-1} \sum_{i=1}^{n} \{\hat{f}_i(x_i) - f(x_i)\}^2 K_2\{(x_i - x_0)/h_2\} ,$$

$$B_n \equiv (nh_2)^{-1} \sum_{i=1}^{n} g(x_i)^{\frac{1}{2}} \epsilon_i \{\hat{f}_i(x_i) - f(x_i)\} K_2\{(x_i - x_0)/h_2\} .$$

Appendix (iv) sketches a proof of (3.4).

The rate of convergence described by (3.1) is optimal. In fact, if the density $d$ is fixed, if $\mathcal{C}(\nu_1, B)$ and $\mathcal{C}_+(\nu_2, B)$ are the function classes defined in Subsection 2.3 but with interval [0,1] replaced by $(-\infty, \infty)$, and if $\hat{g}$ is any nonparametric estimator of $g$, then for some $C > 0$,

$$\liminf_{n\to\infty} \sup_{f\in\mathcal{C}(\nu_1,B), g\in\mathcal{C}_+(\nu_2,B)} P_{f,g}\{|\hat{g}(x_0) - g(x_0)| > C \max(n^{-\nu_2/(2\nu_2+1)}, n^{-2\nu_1/(2\nu_1+1)})\} > 0 .$$

This is an analogue of (2.13), and has an almost identical proof.

All the results above have versions for parametric estimation of $g$, corresponding to $\nu_2 = \infty$. In this circumstance we usually do not require parametric knowledge about the design density $d$, since parametric estimation of $g$ does not involve estimation of $d$. It is usually sufficient to ask that $d$ be $\nu_1$-smooth.

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*Appendix (i): Proof of (2.4) and (2.5).*

Since $\hat{f}$ is defined by interpolation from $\hat{f}(i/n)$, it suffices to show that

$$\sup_{\delta n\le i\le n-\delta n} |E\hat{f}(i/n) - f(i/n)| = O\{(nh_1)^{-\nu_1}\} , \sup_{n\le i\le n-\delta n} \mathrm{var}\{\hat{f}(i/n)\} = O(h_1) . \tag{A.1}$$

Observe from definition (2.3) and properties of $\{a_k\}$ that

$$E\hat{f}(i/n) - f(i/n) = \Sigma_k a_k(\langle\nu_1\rangle!)^{-1}(k/n)^{\langle\nu_1\rangle}[f^{(\langle\nu_1\rangle)}\{(i+\theta_k k)/n\} - f^{(\langle\nu_1\rangle)}(i/n)]\,,$$

where $0 \le \theta_k \le 1$. Since $f$ is $\nu_1$-smooth then $|f^{(\langle\nu_1\rangle)}(x) - f^{(\langle\nu_1\rangle)}(y)| \le C_1|x-y|^{\nu_1 - \langle\nu_1\rangle}$, from which it follows that

$$\begin{aligned}|E\hat{f}(i/n) - f(i/n)| &\le C_1\Sigma_k|(k/n)^{\langle\nu_1\rangle}a_k|\,|k/n|^{\nu_1-\langle\nu_1\rangle}\\ &= C_1 n^{-\nu_1}\Sigma_k|k|^{\nu_1}|a_k| \le C_2(nh_1)^{-\nu_1}\,,\end{aligned}$$

which gives the first part of (A.1). The second part follows from

$$\operatorname{var}\{\hat{f}(i/n)\} = \Sigma a_k^2 g\{(i+k)/n\} \le (\sup g)\Sigma a_k^2 = O(h_1)\,.$$

*Appendix (ii): Proof of (2.10).*

Put $D_i \equiv E\hat{f}(i/n) - f(i/n)$, $\Delta_i \equiv \Sigma_k a_k g\{(i+k)/n\}^{\frac{1}{2}}\epsilon_{i+k}$. Then $\hat{r}_i = g(i/n)^{\frac{1}{2}}\epsilon_i - D_i - \Delta_i$, so that $\hat{g}(i/n) - g(i/n) = \Sigma_{1\le j\le 6}S_j$, where

$$S_1 \equiv \Sigma_l b_l g\{(i+l)/n\}(\epsilon_{i+l}^2 - 1)\,,\quad S_2 \equiv \Sigma_l b_l D_{i+l}^2\,,\quad S_3 \equiv \Sigma_l b_l \Delta_{i+l}^2\,,$$

$$S_4 \equiv -2\Sigma_l b_l g\{(i+l)/n\}^{\frac{1}{2}} D_{i+l}\epsilon_{i+l}\,,\quad S_5 \equiv -2\Sigma_l b_l g\{(i+l)/n\}^{\frac{1}{2}}\epsilon_{i+l}\Delta_{i+l}\,,$$

$$S_6 \equiv 2\Sigma_l b_l D_{i+l}\Delta_{i+l}\,.$$

It suffices to show that

$$\sup_{\delta n\le i\le n-\delta n,\,1\le j\le 6}\left[\{ES_j(i)\}^2 + \operatorname{var} S_j(i)\right] = O\{h_2 + (nh_2)^{-2\nu_2} + h_1^2 + (nh_1)^{-4\nu_1}\}\,. \quad (A.2)$$

Observe that $E(S_j) = 0$ for $j = 1,4$ and 6; $|D_i| = O\{(nh_1)^{-\nu_1}\}$, by (A.1); $E(\Delta_i^2) = O(\Sigma a_k^2) = O(h_1)$; and $E(\epsilon_i\Delta_i) = a_0 g(i/n) = O(h_1)$. Therefore $E(S_2) = O\{(nh_1)^{-2\nu_1}\}$, $E(S_3) = O(h_1) = E(S_5)$. Hence, each $(ES_j)^2$ admits the bound claimed in (A.2). Trivially, $\operatorname{var}(S_1) = O(\Sigma b_l^2) = O(h_2)$, $\operatorname{var}(S_2) = 0$, $\operatorname{var}(S_4) = O(\Sigma b_l^2) = O(h_2)$. Furthermore,

$$\begin{aligned}E(S_3^2) = \Sigma_{l_1}\Sigma_{l_2}\Sigma_{k_1}\ldots\Sigma_{k_4} b_{l_1}b_{l_2}a_{k_1}\ldots a_{k_4}&\big[g\{(i+l_1+k_1)/n\}g\{(i+l_1+k_2)/n\}\\ \times g\{(i+l_2+k_3)/n\}g\{(i+l_2+k_4)/n\}\big]^{\frac{1}{2}}&E(\epsilon_{i+l_1+k_1}\epsilon_{i+l_1+k_2}\epsilon_{i+l_2+k_3}\epsilon_{i+l_2+k_4})\,.\end{aligned}$$

The expectation on the right-hand side vanishes unless either $k_1 = k_2$ and $k_3 = k_4$; or $l_1 - l_2 = k_3 - k_1 = k_4 - k_2$; or $l_1 - l_2 = k_4 - k_1 = k_3 - k_2$. In the first case, all nonzero terms except those corresponding to $k_1 = k_2 = k_3 = k_4$, cancel perfectly from the difference $E(S_3^2) - (ES_3)^2$; and in the second and third cases, once $l_1, l_2, k_1$ and $k_2$ are given, $k_3$ and $k_4$ are completely determined. Therefore, since $|a_k| \le C_1 h_1$,

$$\begin{aligned}\operatorname{var}(S_3) &\le C_2\left(\Sigma_{l_1}\Sigma_{l_2}\Sigma_k|b_{l_1}b_{l_2}a_k|h_1^3 + \Sigma_{l_1}\Sigma_{l_2}\Sigma_{k_1}\Sigma_{k_2}|b_{l_1}b_{l_2}a_{k_1}a_{k_2}|h_1^2\right)\\ &= O(h_1^2)\,.\end{aligned}$$

Similar but simpler arguments show that $\operatorname{var}(S_5) = O(h_1^2+h_2)$, $\operatorname{var}(S_6) = O\{h_1(nh_1)^{-2\nu_1}\}$. Hence, each $\operatorname{var}(S_j)$ admits the bound claimed in (A.2).

*Appendix (iii): Proof of (2.15).*

We may assume that $\nu_1 \le \frac{1}{2}$ and $\nu_2 \ge \nu_1$, for otherwise (2.15) follows from (2.14). For simplicity we further suppose that $B > 2$. Let $\psi$ be a nondegenerate, twice-differentiable function on $(-\infty, \infty)$ satisfying $\psi(x) = 0$ for $x \le 0$ and $x \ge 1$, and $\sup|\psi'| \le 1$. Fix $c_1 > 0$, and write $m_1, m$ for integers such that $m_1 \sim c_1 n^{2\nu_1/(2\nu_1+1)}$, $m_1 m \le n$ and $m_1 m \sim n$. Then $m \sim c_1^{-1} n^{1/(2\nu_1+1)}$. Put $\delta_1 \equiv m_1/n$ and $\delta \equiv \delta_1^{2\nu_1}$. Let $I_1, \ldots, I_m$ be a sequence of 0's and 1's, and define $f = f(\cdot \mid I_1, \ldots, I_m)$ by

$$\begin{aligned} f\left[\{(i-1)m_1 + j\}/n\right] &= \delta^{\frac{1}{2}} I_i \psi(j/n\delta_1) \quad \text{if } 1 \le i \le m \text{ and } 1 \le j \le m_1\,, \\ f(x) &= 0 \quad \text{if } x \le 0 \text{ or } x \ge m_1 m/n\,. \end{aligned} \tag{A.3}$$

Write $\mathcal{F}$ for the set of all such $f$'s. Define constant functions $g_0 \equiv 1$ and $g_1 \equiv 1 + c_2\delta$, where $c_2 \ne 0$, and let $\mathcal{G} = \{g_0, g_1\}$. For large $n$, $\mathcal{F} \subseteq C(\nu_1, B)$ and $\mathcal{G} \subseteq C_+(\nu_2, B)$.

We claim that if $0 < x_0 < 1$ and $\hat{g}$ is a nonparametric estimator of $g$,

$$\sup_{f\in\mathcal{F}, g\in\mathcal{G}} E_{f,g}\{\hat{g}(x_0) - g(x_0)\}^2 \ge C n^{-4\nu_1/(2\nu_1+1)}\,, \tag{A.4}$$

where $C > 0$. It suffices to prove this result for estimators which are functions of $Y_i$ for $i \le m_1 m$. Let $I_1, \ldots, I_m$ be independent symmetric 0–1 variables, independent also of the

$\epsilon_i$'s. For these $I_i$'s, write $f^*$ for the (random) function defined as $f$ at (A.3), and let $J$ denote the likelihood ratio rule for discriminating between the hypotheses

$$H_0 : Y_i = f^*(i/n) + g_0(i/n)^{\frac{1}{2}}\epsilon_i\,, \quad H_1 : Y_i = f^*(i/n) + g_1(i/n)^{\frac{1}{2}}\epsilon_i\,.$$

Define $\hat{J} = 0$ if $|\hat{g}(x_0) - g_0(x_0)| \le |\hat{g}(x_0) - g_1(x_0)|$, and $\hat{J} = 1$ otherwise. Write $P_i$ and $E_i$ for probability and expectation under $H_i$. Then

$$\begin{aligned}\sup_{f\in\mathcal{F},g\in\mathcal{G}} E_{f,g}\{\hat{g}(x_0) - g(x_0)\}^2 &\ge \max_{i=1,2} E_i\{\hat{g}(x_0) - g_i(x_0)\}^2 \\ \ge (\tfrac{1}{2}c_2\delta)^2 \max\{P_0(\hat{J}=1), P_1(\hat{J}=0)\} &\ge \tfrac{1}{8}(c_2\delta)^2\{P_0(\hat{J}=1) + P_1(\hat{J}=0)\} \\ &\ge \tfrac{1}{8}(c_2\delta)^2\{P_0(J=1) + P_1(J=0)\}\,,\end{aligned}$$

by the optimality of the likelihood ratio rule. Therefore (A.4) will follow if we prove

$$\liminf_{n\to\infty} P_0(J=1) > 0\,. \tag{A.5}$$

Let $(g, H)$ denote either $(g_0, H_0)$ or $(g_1, H_1)$. If $k = (i-1)m_1 + j$ where $1 \le i \le m$ and $1 \le j \le m_1$, write $Y_{ij}$ for $Y_k$ and $\epsilon_{ij}$ for $\epsilon_k$. Assuming standard normal errors $\epsilon_{ij}$, the likelihood of $H$ given $Y_1, \ldots, Y_{m_1m}$ is proportional to

$$L(H) \equiv g^{-m_1m/2}\prod_{i=1}^{m}\left(\exp\left(-\tfrac{1}{2}g^{-1}\sum_{j=1}^{m_1}Y_{ij}^2\right) + \exp\left[-\tfrac{1}{2}g^{-1}\sum_{j=1}^{m_1}\{Y_{ij} - \delta^{\frac{1}{2}}\psi(j/n\delta_1)\}^2\right]\right).$$

If $H_0$ is true then

$$\begin{aligned}L(H) &= g^{-m_1m/2}\exp(-\tfrac{1}{2}g^{-1}\Sigma_i\Sigma_j\epsilon_{ij}^2) \\ &\times \Pi_i\left[\exp\{-\tfrac{1}{2}I_i(d_1 + 2d_1^{\frac{1}{2}}N_i)g^{-1}\} + \exp\{-\tfrac{1}{2}(1-I_i)(d_1 - 2d_1^{\frac{1}{2}}N_i)g^{-1}\}\right],\end{aligned}$$

where $d_1 \equiv \delta\Sigma_j\psi^2(j/n\delta_1) \sim d \equiv c_1^{2\nu_1+1}\int\psi^2$, and $N_i \equiv d_1^{-\frac{1}{2}}\delta^{\frac{1}{2}}\Sigma_j\psi(j/n\delta_1)\epsilon_{ij}$ is standard normal. Therefore, using the symmetry of $N_i$,

$$R \equiv 2\log\{L(H_1)/L(H_0)\} = m_1m(1 - g_1^{-1} + \log g_1^{-1}) - 2(g_1^{-1} - 1)mD + o_p(m_1m\delta^2 + m\delta)\,,$$

where $D \equiv E[\{1 + \exp(\frac{1}{2}d + d^{\frac{1}{2}}N_1)\}^{-1}(\frac{1}{2}d + d^{\frac{1}{2}}N_1)]$. Note that

$$|g_1^{-1} - 1||\Sigma_i\Sigma_j(\epsilon_{ij}^2 - 1)| = O_p\{(m_1m\delta^2)^{\frac{1}{2}}\} = o_p(m_1m\delta^2)\,.$$

Choose $c_1$ so that $D \neq 0$, let $c_3 > 0$ and put $c_2 \equiv c_3 \operatorname{sgn}(D)$. Since $g_1 = 1 + c_2\delta$ then

$$R = -\tfrac{1}{2}m_1 m\delta^2 c_3^2\{1 + o_p(1)\} + m\delta c_3|D|\{1 + o_p(1)\} .$$

Choose $c_3$ so small that $c_4 \equiv c_3|D| - \frac{1}{2}c_1^{2\nu_1+1}c_3^2 > 0$. Then $R \sim c_4 m\delta \to \infty$, so that $P_0(J = 1) \to 1$, proving (A.5).

*Appendix (iv): Sketch proof of (3.4).*

Let $s(x) \equiv f(x)\,d(x)$ and $\hat{s}_i(x) \equiv \hat{f}_i(x)\hat{d}_{1i}(x)$. Assume $\nu_1 > \nu_2/\{2(\nu_2 + 1)\}$, and put $\xi_n \equiv \max(n^{-2\nu_1/(2\nu_1+1)}, n^{-2\nu_2/(2\nu_2+1)})(\log n)^2$. Equation (3.4) will follow if $|A_n| = O_p(\xi_n)$, $|B_n| = O_p(\xi_n)$. Dropping the argument $x$,

$$\begin{aligned}
\hat{f}_i - f &= (\hat{s}_i - s)/d - (\hat{s}_i - s)(\hat{d}_{1i} - d)/(d\hat{d}_{1i}) - s(\hat{d}_{1i} - d)/(d\hat{d}_{1i}) \\
&= (\hat{s}_i - s)/d - (\hat{s}_i - s)(\hat{d}_{1i} - d)/(d\hat{d}_{1i}) - s(\hat{d}_{1i} - d)/d^2 \\
&\quad + s(\hat{d}_{1i} - d)^2/(d^2\hat{d}_{1i}) . \qquad \text{(A.6)}
\end{aligned}$$

For $A_n$, note that

$$(\hat{f}_i - f)^2 \leq 10\{(\hat{s}_i - s)^2/d^2 + (\hat{s}_i - s)^2(\hat{d}_{1i} - d)^2/(d\hat{d}_{1i})^2 + (s/d)^2(\hat{d}_{1i} - d)^2/\hat{d}_{1i}^2\} .$$

This bounds $A_n$ by the sum of three terms, say $A_{n1}$, $A_{n2}$ and $A_{n3}$. By (3.3), $A_{n3} = O_p(\xi_n)$. If we show that $A_{n1} = O_p(\xi_n)$, the same easily follows for $A_{n2}$ by (3.3). Define

$$\begin{aligned}
v_1(x_i) &\equiv (nh_1)^{-1}\sum_{k\neq i}\{f(x_k) - f(x_i)\}K_1\{(x_k - x_i)/h_1\}/d(x_i) , \\
v_2(x_i) &\equiv (nh_1)^{-1}\sum_{k\neq i} g(x_k)^{\frac{1}{2}}\epsilon_i K_1\{(x_k - x_i)/h_1\}/d(x_i) , \\
v_3(x_i) &\equiv f(x_i)\{\hat{d}_{1i}(x_i) - d(x_i)\}/d(x_i) .
\end{aligned}$$

Since $Y_k - f(x_i) = f(x_k) - f(x_i) + g(x_k)^{\frac{1}{2}}\epsilon_k$ then $A_{n1} \leq A_{n11} + A_{n12} + A_{n13}$, where

$$A_{n1j} = 10(n\delta_2)^{-1}\sum_{i=1}^{n}|K_2\{(x_i - x_0)/\delta_2\}|v_j^2(x_i) .$$

By (3.3) for the last and moment calculations for the first two, it is seen that each $A_{n1i} = O_p(\xi_n)$.

To study $B_n$, split it into four terms $B_{n1} + B_{n2} + B_{n3} + B_{n4}$ based on (A.6). Using (3.3), $B_{n4} = O_p(\xi_n)$. Since $EB_{n3} = 0$, one proves that $B_{n3} = O_p(\xi_n)$ by showing that $\mathrm{var}\,(B_{n3}) = O(\xi_n^2)$, which is an easy calculation. For $B_{n2}$ apply Cauchy-Schwarz, (3.3) and the arguments used to bound $A_{n1}$, to show that $B_{n2} = O_p(\xi_n)$. This leaves us to study $B_{n1}$. Now $B_{n1} = B_{n11} + B_{n12} + B_{n13}$, where

$$B_{n1j} = (nh_2)^{-1} \sum_{i=1}^{n} g(x_i)^{\frac{1}{2}} \epsilon_i K_2\{(x_i - x_0)/h_2\} v_j(x_i)\,.$$

Each of these random variables has mean zero and variance $O(\xi_n^2)$, completing the proof.

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